Industrial and Engineering Chemistry Research 2015 vol.54 N40, pages 9850-9856

Building Blocks for Ionic Liquids: Vapor Pressures and Vaporization Enthalpies of N-Functionalized Imidazoles with Branched and Cycloalkyl Substituents

Verevkin S., Zaitseva K., Stanton A., Hindman M., Irvin A., Bara J.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 American Chemical Society. The imidazole structure offers a versatile means of developing molecules with controlled/tunable physicochemical properties that have significant utility in many applications and can be further derivatized to form ionic liquids. In the literature, the vast majority of studies on structure-property relationships in these types of molecules are devoted to linear (e.g., n-alkyl) substituents. However, imidazoles with branched or cycloalkyl groups are equally accessible through convenient synthetic methods - yet there are essentially no reports on the physical properties of such compounds in the literature. Here, the absolute vapor pressures of branched and cycloalkyl derivatives of imidazole have been determined as a function of temperature by the transpiration method. The standard molar enthalpies of vaporization were derived from the temperature dependences of vapor pressures. The measured data sets were successfully checked for internal consistency by comparison with vaporization enthalpies of the parent species, and a group contribution method is put forth by which the vaporization enthalpies of imidazoles, and imidazolium-based ILs, with alkyl groups in any configuration can be rapidly predicted.

http://dx.doi.org/10.1021/acs.iecr.5b01599